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APPLICATION OF FLUENT TO PREDICT COMBUSTION PERFORMANCE FOR PURE PROPANE

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of the requirements for the award of the degree of
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ABSTRACT

Computational Fluid Dynamic (CFD) is a used tool in optimizing propane burner for emissions issues and to study combustions characteristics of flame temperature and flame velocity in furnace system. Using CFD simulation, cost and time can reduce in development new furnace and burner. Studies are aimed at improving combustion performance with reduce pollutant emissions. Also focus on the combustion patterns in the form of measured contours of temperature and species concentrations. Pure propane used as a fuel in this research. Before doing computer simulation, several experiments were running first. Only the best data will choose. This data is use in boundary setting when doing simulation process. In experimental work, practical combustor C492 gas burner is used. The data from the experimental work will analyze and compare to get a constant and stable data. For simulation work 2D design for practical combustor was done in Gambit software. In this software, the design was mesh and export to Fluent 6.3. Fluent 6.3 is one of CFD software that uses to study combustion and flow characteristics. The result from experimental work and computer simulation then compared. The comparison shows in the Table 4.2 in term of percentage differences. Best result depends on small percentage between this two data.

ABSTRAK

Pengaturcaraan Computational Fluid Dynamic (CFD) digunakan untuk mendapatkan kesan pencemaran dan ciri-ciri pembakaran seperti suhu dan halaju api di dalam sistem pembakar gas propana. Penggunaan CFD juga dapat menjimatkan masa dan kos di dalam pembinaan pembakar (furnace) baru. Ujikaji ini difokuskan kepada peningkatan prestasi pembakaran disamping mengurangkan pencemaran. Ia juga bagi mendapatkan bentuk gambar perubahan suhu dan kepekatan spesis hasil daripada pembakaran. Gas propana (tulen) digunakan sebagai bahan bakar. Sebelum simulasi menggunakan komputer dilakukan, beberapa ujikaji makmal dilakukan menggunakan pembakar dari model C492 yang sedia ada. Data daripada beberapa ujikaji dianalisa dan dibuat perbandingan bagi mendapatkan data yang malar dan stabil. Untuk kerja-kerja simulasi pembakar dari jenis jenis C942 akan dilukis secara 2 dimensi di dalam perisian Gambit. Kemudian hasil lukisan itu akan dimasukkan ke dalam perisian Fluent 6.3. untuk mendapatkan hasil simulasi, data yang dikumpulkan daripada ujikaji makmal akan dibandingkan dengan data yang dikumpul hasil proses simulasi. Perbezaan data dapat dilihat di dalam Jadual 4.2 dalam bentuk peratusan. Peratusan yang kecil adalah hasil yang terbaik.

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LIST OF SYMBOLS

n_c	-	Combustion efficiency
$\mathbf{v}$	-	Mean fluid velocity
D	-	Characteristic diameter
μ	-	Dynamic fluid viscosity
ν	-	Kinematic fluid viscosity
ρ	-	Density
λ	-	Second viscosity coefficient
δij	-	Kronecker delta
$\Sigma\nabla.\mathbf{u}$	-	Divergence
$\Sigma\mu B$	-	Black viscosity
P	-	Pressure of the system
V	-	Volume of the gas
K	-	Constant value representative pressure and volume
T	-	Temperature
α	-	Cubic expansivity
n	-	Number of mole
R	-	Universal gas constant
u'	-	Root mean square of turbulent velocity fluctuation
U	-	Mean velocity
Re_{d_h}	-	Reynolds number based on the pipe hydraulic diameter
d_h	-	Hydraulic diameter

a	-	Width
b	-	Height
d_i	-	Inner diameter
d_o	-	Outer diameter
CFD	-	Computational Fluid Dynamic
2D	-	Two dimension

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CHAPTER 1

INTRODUCTION

1.1 Introduction

A furnace is a device that produces heat. Not only are furnaces used in the home for warmth, they are used in industry for a variety of purposes such as making steel and heat treating of materials to change their molecular structure.

Central heating with a furnace is an idea that is centuries old. One of the earliest forms of this idea was invented by the Romans and called a hypocaust. It was a form of under-floor heating using a fire in one corner of a basement with the exhaust vented through flues in the walls to chimneys. This form of heating could only be used in stone or brick homes. It was also very dangerous because of the possibility of fire and suffocation.

Furnaces generate heat by burning fuel, but early furnaces burned wood. In the seventeenth century, coal began to replace wood as a primary fuel. Coal was used until the early 1940s when gas became the primary fuel. In the 1970s, electric furnaces started to replace gas furnaces because of the energy crisis. Today, the gas furnace is still the most popular form of home heating equipment.

Wood and coal burning furnaces required constant feeding to maintain warmth in the home. From early morning to late at night, usually three to five times a day, fuel needed to be put in the furnace. In addition, the waste from the ashes from the burnt wood or coal must be removed and disposed.

Today's modern furnace uses stainless steel, aluminized steel, aluminum, brass, copper, and fiberglass. Stainless steel is used in the heat exchangers for corrosion resistance. Aluminized steel is used to construct the frame, blowers, and burners. Brass is used for valves, and copper in the electrical wiring. Fiberglass is used insulate the cabinet.

1.2 Background of Study

An industrial furnace or direct fired heater, is an equipment used to provide heat for a process or can serve as reactor which provides heats of reaction. Furnace designs vary as to its function, heating duty, type of fuel and method of introducing combustion air. However, most process furnaces have some common features.

Fuel flows into the burner and is burnt with air provided from an air blower. There can be more than one burner in a particular furnace which can be arranged in cells which heat a particular set of tubes. Burners can also be floor mounted, wall mounted or roof mounted depending on design. The flames heat up the tubes, which in turn heat the fluid inside in the first part of the furnace known as the radiant section or firebox. In this chamber where combustion takes place, the heat is transferred mainly by radiation to tubes around the fire in the chamber. The heating fluid passes through the tubes and is thus heated to the desired temperature. The gases from the combustion are known as flue gas. After the flue gas leaves the firebox, most furnace designs include a convection section where more heat is recovered before venting to the atmosphere through the flue gas stack. HTF=Heat Transfer Fluid. Industries commonly use their furnaces to heat a secondary fluid with special additives like anti-rust and high heat transfer efficiency. This heated fluid is then circulated round the whole plant to heat exchangers to be used wherever heat is needed instead of directly heating the product line as the product or material may be volatile or prone to cracking at the furnace temperature. [1]

A computer code for simulating combustion gas flow is a powerful tool in the initial stage of combustor design. Currently there are various commercial computational fluid dynamics (CFD) codes in the market. One of the CFD's software is FLUENT 6.3. FLUENT 6.3 is a computational fluid dynamics (CFD) software package to simulate combustion process. Using FLUENT 6.3 a study for flame temperature, flue gases, velocity vector and concentration of the combustion products can be developed.

The simulation process for this research will continued with experimental study. The experimental work will use a standard C492 gas burner. The gas burner is a device to burn fuels under control to produce useful heat. Function of the burner are to deliver fuel and air to a combustion chamber, mix fuel and air, and provide continuous and stable ignition of air/fuel mixture. For this project pure propane used as a fuel for combustion. Result from experimental work and CFD simulation will compare, and then analyze.

1.3 Problem Statement

Computational fluid dynamics (CFD) has proven being a valuable tool in optimizing combustion equipments and gas burners. Using CFD simulation, is easy to get accurate data measurement. It is also reduces the times and cost of development new burner. The main reason for doing the simulation is the measurement of the detailed distributions of velocity, temperature and gas composition are very difficult for practical combustor. In this study, therefore, the numerical simulation for the prediction of local combustion properties of pure propane by the standard C492 gas burner in the experimental combustor is described. The accuracy of the simulation is discussed by comparing of the calculated and measured results.

1.4 Objective of the Project

The objective of the project is to develop a CFD simulation to predict combustion performance for pure propane in term of emissions, flame temperature, velocity vectors and concentration of the combustion products, and validate with experimental data.

1.5 Scope of Research Work

The scopes of research are:

1. To mesh the 2D drawing of C492 gas burner in Gambit.
2. To develop the CFD simulation using FLUENT 6.3 software.
3. To compare the expected result from simulation with experimental work.

1.6 Thesis Organization

This thesis consists of five chapters summarized as follows:

Chapter 2 comprises a literature survey on the subject of combustion performance using CFD simulation. This chapter briefly discuss about the natural gas combustion and CFD simulation.

Chapter 3 concentrates on the methodology of this research, flowchart, experimental setup instrumentation and measurement.

Chapter 4 provides the result from experimental work and simulation process.

Chapter 5 summaries the results and provides conclusions and recommendation for future work.

CHAPTER 2

LITERATURE RIVIEW

2.1 Introduction

The purpose of this chapter is to provide a review of past research effort related to furnace, gas burner, combustion, computational fluid dynamics (CFD) analysis, two dimensional and three dimensional modeling. A review of other relevant research studies is also provided. Substantial literature has been studied on experimental and numerical study. However, little information can be found on formulated how to applied the boundary condition (BC) from experimental data to the three dimensional modeling analysis. The review is organized chronologically to offer insight to how past research efforts have laid the groundwork for subsequent studies, including the present research effort. The review is detailed so that the present research effort can be properly tailored to add the present body of literature as well as to justify the scope and direction of the present research effort.

2.2 Combustion

All of uses are dependent on the combustion of fossils fuels, whether for generating electricity, heating domestic water, or within an internal combustion engine. As they are a finite resource, using them efficiently and with minimum pollution is increasingly important.

Combustion is a chemical reaction (oxidisation) between combustible components of the fuel and oxygen in the air. The reaction is rapid and heat, light and energy are released as flame, which one started by an ignition source, is self-propagating. The process requires a substance that will burn, and this is usually a fossil fuel, such as coal, oil and gas. They contain a mixture of hydrogen and carbon and so are known as hydrocarbons.

For each hydrocarbon fuel there is a chemical equation of the reactants (fuel and air) forming the product of combustion. From this the theoretical air to fuel ratio can be determined as well as the constituents of the products of combustion.

In perfect combustion of hydrocarbons all the hydrogen and carbon in the fuel are oxidised to produce mainly carbon dioxide (CO_2) and water (H_2O), although there may be small amounts of carbon monoxide and partially reacted flue constituents. This is call stoichiometric combustion where the exact theoretical air quantity is supplied. Therefore the exhaust gas contains neither incompletely oxidised fuel constituents nor oxygen. So this means the CO_2 in the flue gas is the maximum attainable.

If insufficient air is supplied, incomplete combustion will result, with part of the fuel remaining unoxidised. This will mean increased levels of carbon monoxide (CO) in the flue gas which can be dangerous and also pollutes the air. In oil burner this will also produce higher smoke number with sooting of the heat transfer surfaces, reducing their effectiveness.

In practice, to ensure complete combustion, excess air is supplied beyond that theoretically required for full oxidization of the fuel. This express as a percentage of the theoretical air needed i.e. 10% excess air is 1.1 times the theoretical air quantity. Having excess air ensures no fuel is wasted, and variations in fuel quality or air and fuel rates can be tolerated and still guarantee complete combustion.

The control of the excess air is the key to combustion efficiency – too little will cause incomplete combustion with the problems mentioned above, whilst too much will cool the combustion chamber and carry a larger percentage of the heat out of the flue, reducing combustion efficiency.

Air consists of 21% oxygen and 79% nitrogen is inert and takes no part in the combustion process. It will enter the appliance at the ambient temperature, and leave through the flue, several hundred degrees higher, wasting heat in the process. This is a basic inefficiency which has to be accepted as there is no economical way of separating the oxygen and nitrogen.

The only reliable way of determining what is happening in a given combustion process is to take a flue gas sample using an analyzer. These vary in complexity, but will have as a minimum an oxygen sensor. Others may have sensors for other gases such as CO, NO and SO. From the oxygen sensor, knowing the particular fuel characteristics, the CO_2 and excess air values can be derived.

2.3 Combustion Efficiency

Failure to achieve high level of combustion efficiency is generally regarded as unacceptable, partly because combustion inefficiency represents a waste of fuel, but mainly because it is manifested in the form of pollutant emissions such as unburned hydrocarbons and carbon monoxide. That is why current emissions regulations call for combustion efficiencies in excess of 99 percents. For the aircraft engine, an additional requirement is that combustion efficiencies should be fairly high, say from 75 to 80 percents, when the engine is being accelerated to its normal rotational speed after a flameout in flight. A high combustion efficiency is necessary at this "off design" point because, with the engine wind milling, the pressure and the temperature of the air flowing through the combustor are close to ambient values. At high altitudes, these are so low that the stability limits are very narrow. This means that when the engine control system attempts to compensate for combustion inefficiency by supplying more fuel to the combustor, this extra fuel may cause a "rich extinction" of the flame. [2]

2.4 Combustion Process

The primary purpose of combustion is to raise the temperature of the airflow by efficient burning of fuel. From a design viewpoint, an important requirement is a means of relating combustion efficiency to the operating variables of air pressure, temperature and mass flow rate, and to the combustor dimensions. Unfortunately, the various process taking place within the combustion zone are highly complex and a detailed theoretical treatment is precluded at this time. Until more information is available, suitable parameters for relating combustion performance to combustor dimensions and operating conditions can be derived only through the use of very simplified models to represent the combustion process. One such model starts from the well establish and widely accepted nation that the total time required to burn a liquid fuel is the sum of the times required for fuel evaporation, mixing of fuel vapor with air and combustion products, and chemical reaction. Because the time available for combustion is inversely proportional to the airflow rate, the combustion efficiency may be expressed as

$$n_c = f\,(\text{airflow rate})^{-1}\ (1/\text{evaporation rate} + 1/\ \text{mixing rate} + 1/\ \text{reaction rate})^{-1}$$

In practical combustion systems, the maximum of heat release under any given operating conditions may be governed by either evaporation, mixing or chemical reaction, but rarely by all three at the same time. However, when the combustion process is in transition from one regime to another, two of the three keys rates will participate in determining the overall combustion efficiency. [2]

2.5 Pure Propane as a Fuel for Combustion

Propane is a three-carbon alkane, normally a gas, but compressible to a transportable liquid. It is derived from other petroleum products during oil or natural gas processing. It is commonly used as a fuel for engines, barbecues, and home heating systems.

When used as vehicle fuel, it is commonly known as liquefied petroleum gas (LPG or LP-gas), which can be a mixture of propane along with small amounts of propylene, butane, and butylene. The odorant ethanethiol is also added so that people can easily smell the gas in case of a leak. [3]

Propane is produced as a byproduct of two other processes: natural gas processing and petroleum refining. The processing of natural gas involves removal of butane, propane and large amounts of ethane from the raw gas to prevent condensation of these volatiles in natural gas pipelines. Additionally, oil refineries produce some propane as a by-product of production of cracking petroleum into gasoline or heating oil. Table 2.1 shows the properties of propane in general.

Propane undergoes combustion reactions in a similar fashion to other alkanes. In the presence of excess oxygen, propane burns to form water and carbon dioxide.

$$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O + \text{heat}$$

Propane + Oxygen → Carbon Dioxide + Water

When not enough oxygen is present for complete combustion, incomplete combustion occurs when propane burns and forms water, carbon monoxide, carbon dioxide, and carbon.

$$C_3H_8 + 3.5\ O_2 \rightarrow CO_2 + CO + C + 4\ H_2O + \text{heat}$$

Propane + Oxygen → Carbon Dioxide + Carbon Monoxide + Carbon + Water

Unlike natural gas, propane is heavier than air (1.5 times as dense). In its raw state, propane sinks and pools at the floor. Liquid propane will flash to a vapor at atmospheric pressure and appears white due to moisture condensing from the air. When properly combusted, propane produces about 50 MJ/kg. The gross heat of combustion of one normal cubic meter of propane is around 91 mega joules

Propane is nontoxic; however, when abused as an inhalant it poses a mild asphyxiation risk through oxygen deprivation. Commercial products contain hydrocarbons beyond propane, which may increase risk. Commonly stored under pressure at room temperature, propane and its mixtures expand and cool when released and may cause mild frostbite.

Propane combustion is much cleaner than gasoline combustion, though not as clean as natural gas combustion. The presence of C-C bonds, plus the multiple bonds of propylene and butylene, create organic exhausts besides carbon dioxide and water vapor during typical combustion. These bonds also cause propane to burn with a visible flame.

Greenhouse gas emissions factors for propane are 62.7 kg CO_2/ mBTU or 1.55 kg of CO_2 per liter or 73.7 kg / GJ.

Table 2.1: Properties of propane

Molecular formula	C_3H_8
Molar mass	44.1 g mol^{-1}
Appearance	Colorless gas
Density	1.83kg/m3,gas 0.5077 kg/L, liquid
Melting point	−187.6 °C (85.5 K)
Boiling point	−42.09 °C (231.1 K)

In this research, pure propane used as fuel. The fuel characteristic from laboratory is 96% propane and 4% mixture of butane, methane and ethane. Appendix A1 use as guideline for safety precaution when running this research.